A global, dynamical formulation of quantum confined systems

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Abstract

A brief review of some recent results on the global self-adjoint formulation of systems with boundaries is presented. We specialize to the 1-dimensional case and obtain a dynamical formulation of quantum confinement.

1 Introduction

Let $H_0 : \mathcal{D}(H_0) \subset L^2(\mathbb{R}^d) \longrightarrow L^2(\mathbb{R}^d)$ be a self adjoint (s.a.) Hamiltonian operator defined on the domain $\mathcal{D}(H_0)$ and describing the dynamics of a d-dimensional quantum system. Let us also consider the decomposition $\mathbb{R}^d =$

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$\Omega \cup \Omega^c$, where Ω is an open set and $\Gamma = \overline{\Omega} \cap \Omega^c$ is the common boundary of the two open sets $\Omega_1 = \Omega$ and $\Omega_2 = \overline{\Omega}^c$.

To obtain a confined version (for instance, to Ω_1) of the system described by H_0, the standard approach is to determine the s.a. realizations of the operator H_0 in $L^2(\Omega_1)$. It is well known, however, that this formulation displays several inconsistencies [1, 2, 3], the main issues being the ambiguities besetting the physical predictions (when there are several possible self-adjoint realizations of H_0 in $L^2(\Omega_1)$), the lack of self-adjoint (s.a.) formulations of some important observables in $L^2(\Omega_1)$ and the difficulties in translating this approach to other (non-local) formulations of quantum mechanics, like the deformation formulation [4]. These problems are well illustrated by textbook examples [1, 4, 5].

Our aim here is to present an alternative approach to quantum confinement. This formulation consists in determining all s.a. Hamiltonian operators $H : \mathcal{D}(H) \subset L^2(\mathbb{R}^d) \longrightarrow L^2(\mathbb{R}^d)$ - defined on a dense subspace $\mathcal{D}(H)$ of the global Hilbert space $L^2(\mathbb{R}^d)$ - which dynamically confine the system to Ω_1 (or Ω_2) while reproducing the action of H_0 in an appropriate subdomain. More precisely, let P_{Ω_k} be the projector operator onto Ω_k, $k = 1, 2$, i.e.

$$P_{\Omega_k}\psi = \chi_{\Omega_k}\psi \quad , \quad \psi \in L^2(\mathbb{R}^d) \tag{1}$$

where χ_{Ω_k} is the characteristic function of Ω_k: $\chi_{\Omega_k}(x) = 1$ if $x \in \Omega_k$ and $\chi_{\Omega_k}(x) = 0$, otherwise. Our aim is to determine all linear operators $H : \mathcal{D}(H) \subset L^2(\mathbb{R}^d) \to L^2(\mathbb{R}^d)$ that satisfy the following three properties:

(i) H is self-adjoint on $L^2(\mathbb{R}^d)$.

(ii) If $\psi \in \mathcal{D}(H)$ then $P_{\Omega_k}\psi \in \mathcal{D}(H)$ and $[P_{\Omega_k}, H]\psi = 0$, $k = 1, 2$.

(iii) $H\psi = H_0\psi$ if $\psi \in \mathcal{D}(H_0)$ is an eigenstate of P_{Ω_k}.

Moreover, for the 1-dimensional case, we want to recast the operators H in the form $H = H_0 + B^{BC}$, where B^{BC} is a distributional boundary potential (that may depend on the particular boundary conditions satisfied by the domain of H) and H is s.a. on its maximal domain. This formulation is global, because the system is defined in $L^2(\mathbb{R}^d)$, and the confinement is dynamical, i.e. it is a consequence of the initial state and of the Hamiltonian H. Indeed, from (i) and (ii) it follows that P_{Ω_k} commutes with all the spectral projectors of H and so also with the operator $\exp\{iHt\}$ for $t \in \mathbb{R}$. Hence, if ψ is an eigenstate of P_{Ω_k} it will evolve to $\exp\{iHt\}\psi$, which is again an eigenstate of P_{Ω_k} with the same eigenvalue. In other words, P_{Ω_k} is a constant of motion and a wave function confined to Ω_1 (or to Ω_2) will stay so forever.

The problem of determining a dynamical formulation of quantum confinement can be addressed from the point of view of the study of s.a. extensions of symmetric restrictions [1, 6, 7, 8] and is closely related with the subjects of point interaction Hamiltonians [7, 9, 10, 11] and surface interactions [12]. Our results may be useful in this last context as well as for the deformation quantization of systems with boundaries [4].

In this paper we shall provide a concise review of the solutions to the above problems. The reader should refer to [13, 14] for a detail presentation, including proofs of the main theorems, the extension of the boundary potential formulation to higher dimensions and some applications to particular systems.

2 Confining Hamiltonians defined on $L^2(\mathbb{R}^d)$

We start by introducing some relevant notation. Let $X, Y \subset V$ be two subspaces of a vector space V such that $X \cap Y = \{0\}$, then their direct sum is denoted by $X \oplus Y$. Let now A, B be two linear operators with domains $\mathcal{D}(A), \mathcal{D}(B) \subset L^2(\mathbb{R}^d)$ such that $\mathcal{D}(A) \cap \mathcal{D}(B) = \{0\}$, then the operator $A \oplus B$ is defined by:

$$A \oplus B : \begin{cases} \mathcal{D}(A \oplus B) = \mathcal{D}(A) \oplus \mathcal{D}(B) \\ = \{\psi \in L^2(\mathbb{R}^d) : \psi = \psi_1 + \psi_2,\, \psi_1 \in \mathcal{D}(A),\, \psi_2 \in \mathcal{D}(B)\} \\ \\ (A \oplus B)\, \psi = A\psi_1 + B\psi_2,\, \forall \psi \in \mathcal{D}(A \oplus B) \end{cases} \tag{2}$$

For simplicity let us assume that $\mathcal{D}(\Omega_k) \subset L^2(\Omega_k) \cap \mathcal{D}(H_0)$, $k = 1, 2$ (where $\mathcal{D}(\Omega_k)$ is the space of infinitely smooth functions $t : \mathbb{R}^d \to \mathbb{C}$ with support on a compact subset of Ω_k) and let us define the operators:

$$H_k^S : \mathcal{D}(\Omega_k) \longrightarrow L^2(\Omega_k),\, \phi \longrightarrow H_k^S \phi = H_0 \phi \quad , \quad k = 1, 2 \tag{3}$$

which are symmetric. Let also $H_k^{S\dagger}$ be the adjoint of H_k^S.

Our main result characterizes the operators $H : \mathcal{D}(H) \subset L^2(\mathbb{R}^d) \to L^2(\mathbb{R}^d)$, associated to a s.a. H_0, and satisfying properties (i) to (iii).

Theorem 1
Let H_0 be s.a. on $L^2(\mathbb{R}^d)$ and such that $\mathcal{D}(H_0) \supset \mathcal{D}(\Omega_1) \cup \mathcal{D}(\Omega_2)$ and

$[H_0, P_{\Omega_k}]\psi = 0$, $k = 1,2$, $\forall\psi \in \mathcal{D}(\Omega_1)\cup\mathcal{D}(\Omega_2)$. An operator H satisfies the defining properties (i) to (iii) iff it can be written in the form $H_1 \oplus H_2$ for some H_1, H_2 s.a. extensions of the restrictions (3). Moreover, all operators H are s.a. extensions of $H_1^S \oplus H_2^S$ and s.a. restrictions of $H_1^{S^\dagger} \oplus H_2^{S^\dagger}$.

The condition (stated in the theorem) that $[H_0, P_{\Omega_k}]\psi = 0$, $\forall\psi \in \mathcal{D}(\Omega_1)\cup\mathcal{D}(\Omega_2)$, and the assumption that H_1^S and H_2^S have s.a. extensions are the minimal requirements for the existence of operators H satisfying (i) to (iii). Proofs of these results are given in [13, 14].

We now focus on the case where $d = 1$, $\Omega_1 = \mathbb{R}^-$ and

$$H_0 = -\frac{d^2}{dx^2} + V(x), \quad \mathcal{D}(H_0) = \{\psi \in L^2(\mathbb{R}) : \psi, \psi' \in AC(\mathbb{R});\ H_0\psi \in L^2(\mathbb{R})\} \tag{4}$$

where $AC(\mathbb{R})$ is the set of absolutely continuous functions on $\mathbb{R}$ and $V(x)$ is a regular potential. We shall assume it to be i) real, ii) locally integrable and satisfying iii) $V(x) > -kx^2$, $k > 0$ for sufficiently large $|x|$. The conditions on $V(x)$ are such that $H_0 : \mathcal{D}(H_0) \subset L^2(\mathbb{R}) \to L^2(\mathbb{R})$ is the unique s.a. realization of the differential expression $-\frac{d^2}{dx^2} + V(x)$ on $L^2(\mathbb{R})$ [15] and ensure that all s.a. realizations of $-\frac{d^2}{dx^2} + V(x)$ on the semi-axes $]-\infty, 0]$ and $[0, +\infty[$ are determined by boundary conditions at $x = 0$ only.

For H_0 of the kind (4) the s.a. operators $H = H_1 \oplus H_2$ are all of the form [13, 15]:

$$H^{\lambda_1,\lambda_2} = H_1^{\lambda_1} \oplus H_2^{\lambda_2} : \begin{cases} \mathcal{D}(H^{\lambda_1,\lambda_2}) = \mathcal{D}(H_1^{\lambda_1}) \oplus \mathcal{D}(H_2^{\lambda_2}) \\ \\ H^{\lambda_1,\lambda_2}\psi = H^{S^\dagger}\psi \end{cases} \tag{5}$$

where

$$\mathcal{D}(H_k^{\lambda_k}) = \{\psi_k = \chi_{\Omega_k}\phi_k :\ \phi_k \in \mathcal{D}(H_0) \wedge \phi_k'(0) = \lambda_k\phi_k(0)\} \tag{6}$$

$\lambda_k \in \mathbb{R}\cup\{\infty\}$, $k = 1,2$ and the case $\lambda_k = \infty$ corresponds to Dirichlet boundary conditions. Moreover

$$H^{S^\dagger} = H_1^{S^\dagger} \oplus H_2^{S^\dagger} : \begin{cases} \mathcal{D}(H^{S^\dagger}) = \{\psi = \chi_{\Omega_1}\phi_1 + \chi_{\Omega_2}\phi_2 :\ \phi_1, \phi_2 \in \mathcal{D}(H_0)\} \\ \\ H^{S^\dagger}\psi = \chi_{\Omega_1}H_0\phi_1 + \chi_{\Omega_2}H_0\phi_2 \end{cases} \tag{7}$$

Hence, all s.a. confining Hamiltonians of the form $H_1 \oplus H_2$ are s.a. restrictions of $H^{S^\dagger}$. To proceed let us define the operators ($k = 1, 2$ and $n = 0, 1$):

$$\hat{\delta}_k^{(n)}(x) : \mathcal{D}(H^{S^\dagger}) \longrightarrow \mathcal{D}'(\mathbb{R});\ \psi = \chi_{\Omega_1}\phi_1 + \chi_{\Omega_2}\phi_2 \longrightarrow \hat{\delta}_k^{(n)}(x)\psi = \delta^{(n)}(x)\phi_k(x) \tag{8}$$

where $\mathcal{D}'(\mathbb{R})$ is the space of Schwartz distributions on $\mathbb{R}$ and $\delta^{(0)}(x) = \delta(x)$ and $\delta^{(1)}(x) = \delta'(x)$ are the Dirac measure and its first distributional derivative. We can now recast the operators (5) in the additive form $H = H_0 + B^{BC}$:

Theorem 2
The s.a. Hamiltonian H^{λ_1,λ_2} given by eq.(5) act as:

$$H^{\lambda_1,\lambda_2}\psi = \left\{ H_0 - B_1^{\lambda_1} + B_2^{\lambda_2} \right\} \psi, \quad \forall \psi \in \mathcal{D}(H^{\lambda_1,\lambda_2}) \tag{9}$$

where now H_0 is the extension to the set of distributions of the original Hamiltonian given in (4), $H_0 : \mathcal{D}'(\mathbb{R}) \longrightarrow \mathcal{D}'(\mathbb{R})$, and

$$B_k^\lambda \equiv \begin{cases} -\hat{\delta}_k'(x) + (-1)^k \hat{\delta}_k(x), & \lambda = \infty \\ \\ \hat{\delta}_k'(x) + 2\lambda\hat{\delta}_k(x) + (-1)^k \frac{d}{dx}\left[\hat{\delta}_k(x) \left(\frac{d}{dx} - \lambda \right) \right], & \lambda \neq \infty \end{cases} \qquad k = 1, 2 \tag{10}$$

Moreover, the maximal domain of the expression (9) coincides with $\mathcal{D}(H^{\lambda_1,\lambda_2})$ (5), i.e.

$$\mathcal{D}_{max}(H^{\lambda_1,\lambda_2}) \equiv \{ \psi \in L^2(\mathbb{R}) :\ H^{\lambda_1,\lambda_2}\psi \in L^2(\mathbb{R}) \} = \mathcal{D}(H^{\lambda_1,\lambda_2}). \tag{11}$$

The proof is given in [13].

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